STALENS

INSIDE

From Dave's Desk

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TWO NOVEL MECHA-NISMS OF DEFORMATION TWINNING IN FACE-CEN-TERED-CUBIC METALS

USING ADVANCED
CHARACTERIZATION
TECHNIQUES TO PROBE
DAMAGE EVOLUTION

CONDENSED MATTER
PHYSICS CONFERENCE
FEATURES PLENARY TALK
BY GRAY

HEADS UP!

New equipment enhances Laboratory's materials capability

MSL home to vertical gas gun for use in dynamic damage nucleation studies

The Materials Science
Laboratory (MSL) has a new
gas gun designed to reliably
shoot in relatively lower
velocity regimes. Scientists
will use this vertical gun,
which stands two stories
tall and has a 10-foot-long
barrel, to study early stage
dynamic damage evolution.

While the Laboratory's traditional facilities are equipped to examine velocity regimes of ~200m/s to more than 1Km/s (peak shock pressures of ~2.5GPa and greater), the ability to reliably shoot in the lower velocity regimes of ~40 to 200m/s (0.5 GPa to 2.5 GPa) hasn't been available at Los Alamos—until now.



Ellen Cerreta (MST-8) and Darcie Dennis-Koller (WX-9) in front of a new, low-speed, gas gun designed to examine the early stages of dynamic damage evolution.

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Taylor anvil impact glovebox for dynamic testing destined for TA-55

The Taylor anvil impact glovebox, to be used for dynamic testing of plutonium and other actinides and completed by IP Systems, Inc. of Broomfield, Colo., was recently delivered to the Materials Science Laboratory.

The Taylor anvil gas gun will be installed within the glovebox, along with the containment chamber, for operational testing in a radiation-free environment before moving it to the TA-55 facilities. Testing will involve proofing of operations within the restrictive limitations imposed by the glovebox and implementing process improvements. The Taylor anvil test involves impacting a right cylinder against an anvil up to several hundred meters per second. This experimental technique

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From Dave's Desk



As the summer draws to a close, I've realized that we have hosted one of the largest groups of students with 33 students performing research in MST Division this summer. I've had the pleasure of meeting several of them and hearing about their research. Many of these students come in with great enthusiasm and energy and I see this spill over to our staff. I would especially like to thank all of our student mentors who put in extra hours and give these students a rewarding, fulfilling, and safe summer research experience. Ensuring a safe working environment often means close supervision, which can be time consuming for the mentors. However, a positive side effect of more face time with your students is that you can teach and mentor them about the science you are performing. For many of our students, this is their first exposure to LANL and ensuring they have a positive experience is important in encouraging them to come back again as a GRA, postdoc or staff scientist as well as going back to their universities and championing that LANL is a great place to do research. Again, thank you mentors for all of your hard work!

I thought it might be useful to give you a little update about the LANL Pressure Safety Program. About a year ago, you probably saw some contractors coming through your labs inventorying pressure equipment, drawing schematics, and developing component lists. Subsequently, Performance Feedback and Improvement Tool (PFITs) issues were issued against many of our systems for being out of compliance. You may have asked yourself what's driving these new changes. In May 2010 the Laboratory issued a new Engineering Standards Manual that specifies new requirements for pressure safety based on DOE orders and OSHA requirements.

Since last fall, I have been heading up an ADEPS directorate-wide committee to develop an implementation plan. Following the example of the electrical safety program, one of the things that



"For many of our students, this is their first exposure to LANL and ensuring they have a positive experience is important in encouraging them to come back again..."

we've done is to establish a training program for pressure safety officers (PSOs). They will be certified to inspect and verify that systems are built and maintained in accordance with LANL requirements. We currently have four in the Division going through the program: Blake Nolen and Joe Wermer (MST-6), James Williams (MST-7), and James Valdez (MST-8). MST-16 will use the TA-55 FOD pressure safety officer resources.

In the coming months, these PSOs will be coming around to your laboratories to help you resolve your pressure safety issues. As system owners, it will be your responsibility to ensure the changes are made and the PSO will help you identify what changes need to be made to put the system into compliance. Please work and cooperate with our PSOs; they have volunteered to help you ensure your pressure systems are safe.

I would like to especially recognize Blake Nolen for taking the initiative of designing a generic manifold design that can be ordered for a reasonable price through Albuquerque Valve and Fitting. The idea is that this manifold will be a LANL-approved manifold and will be delivered to your laboratory fully certified. We're currently working with the gas plant and the pressure safety program to determine how exactly to implement this, but we expect to have it in place in the next 6-12 months. Standardizing our pressure gas manifolds will be a more efficient way of certifying our systems rather than going through a customized certification for each system.

In FY12 we will be pushing hard to close approximately 200 PFITs issues in the Division and certifying many of these systems during that process. But this can't be done by the PSOs themselves. We need your cooperation and involvement to make this a success. If you have any questions about the LANL Pressure Safety Program, please contact your PSOs or you may also contact Jim Coy or me.

MST Deputy Division Leader Dave Teter

Vertical... Recent studies of dynamic damage to support advanced damage models have demonstrated the need to understand damage evolution that occurs at these relatively lower peak shock pressures and to correlate with surrounding microstructure. This new gas gun platform, with catch tank, will make it possible for scientists to soft recover specimens for postmortem characterization and to obtain in situ diagnostic data from experiments.

The Laboratory has only one other vertical gas gun, at TA-55, but it has a different function. It fires from the bottom up, instead of the top down, as is the case with the new gas gun at the Materials Science Laboratory.

In a collaborative effort, Shock and Detonation Physics (WX-9) and Structure/Property Relations (MST-8) researchers established this capability for low velocity shock loading experiments. Spearheading the project were Darcie Dennis-Koller (WX-9) and Ellen Cerreta, Carl Trujillo, Daniel Martinez, Juan Pablo Escobedo (MST-8). The Los Alamos Laboratory Directed Research and Development program sponsored this project. Physics Applications designed and built the gun to specification.

Technical Contact: Carl Trujillo

Taylor... is currently used to validate constitutive strength and damage models for a variety of metals, polymers, and composites under high strain rate impact conditions (including transient shock waves) and multi-axial stress conditions. Metallographic characterization is used to understand the resulting deformation microstructures, how the microstructures evolve, and how the microstructures affect the deformation behavior. Applied to plutonium, the Taylor anvil capability is a critical link between small-scale fundamental experiments (such as the Kolsky bar, quasi-static compression, and the 40-mm gas gun) and costly, large-scale, high-pressure, integrated plutonium experiments. Tests provide direct experimental validation of computer simulations performed by T, WT, and X Divisions using advanced strength, damage, and equation-of-state models to accurately predict the mechanical response of plutonium.

Manny Lovato and Bill Blumenthal (MST-8) and Paul Contreras, George Kaschner, and Paula Crawford (Nuclear Materials Science, MST-16) have worked with Chris Roybal, Paul Herrera (Applied Engineering Technology, AET-5), and Kevin Van Cleave (Project Engineering Office, ES-PE), to successfully complete the design and fabrication of the Taylor anvil glovebox. Campaigns 2, 8, and 12 provided support to develop this capability.

Technical contact: Paula Crawford



Taylor anvil glovebox undergoing final acceptance testing at IP Systems, Inc. Manny Lovato (MST-8) is shown evaluating the alignment of the system.

Two novel mechanisms of deformation twinning in face-centered-cubic metals

Researchers Jian Wang (MST-8), Irene J Beyerlein (Physics and Chemistry of Materials, T-1), and Nan Li, Amit Misra, Nathan Mara (Center for Integrated Nanotechnologies, MPA-CINT), for the first time recently reported two novel twinning mechanisms in face-centered-cubic crystal. One is zero-strain twinning and de-twinning mechanism in single phase and the other is interface-facilitated twinning mechanisms in composites. This study provides new insight in understanding deformation mechanisms in fcc crystals and opens a new window in controlling twins in composites.

Crystal twinning results in an intergrowth of two separate crystals in a variety of specific configurations. A twin boundary separates the two crystals. There are three modes of formation of twinned crystals: growth twins, annealing or transformation twins, and deformation or gliding twins. Deformation twinning is a typical deformation mechanism, accomplished by the glide of twinning dislocations. The presence of twin boundaries can strength materials in the order of ten times higher in nanotwinned copper (Cu) due to the discontinuity of slip systems. However it is difficult in single-phase face-centered-cubic metals with medium to high stacking fault energies. Therefore twinning in these cases usually requires extreme conditions, such as shock and/or cryogenic temperatures.

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Deformation... Figure 1 shows the atomistic structure of the incoherent twin boundary (ITB) in Cu by high-resolution transmission electron microscopy (HRTEM) and molecular statics modeling [Appl. Phys. Lett. 95 021908 (2009)]. The HRTEM micrograph of Σ 3{112} ITBs reveals that the atomic structure has a regular repeatable pattern with a unit containing three {111} planes, which corresponds to a set of Shockley partial dislocations with a repeatable sequence b2:b1:b3 on every {111} plane. A noteworthy characteristic of the three partial dislocations is that the sum of their Burgers vectors in one unit equals zero [Acta Mater. 58: 2262]. In situ transmission electron microscopy (TEM) observation and atomistic simulations both synthesize the zero-strain twinning and de-twinning mechanism, in which twinning or de-twinning can be accomplished through the collective glide of Σ 3{112} ITBs, as shown in Figure 2 [Acta Mater. 58: 2262 (2010); Phys. Rev. Lett. **106**: 175504 (2011)].

By virtue of the interface, the researchers recently proposed and demonstrated the interface-facilitated twinning mechanism, particularly for the materials that are hard twinned. Silver (Ag)-Cu eutectic-layered composites are synthesized via a flux-melting technique and then rolled. They found that the Ag-Cu interface facilitates extensive deformation twinning in Cu during room temperature, low strain-rate loading conditions. In this way, twins in Ag can provide an ample supply of twinning partials to Cu to support and sustain twin growth in Cu during deformation. Atomistic simulations reveal that this "ideal" Ag-Cu interface allows transmission of twinning partials from the Ag phase into the Cu phase. As a consequence, the proposed twin nucleation and growth

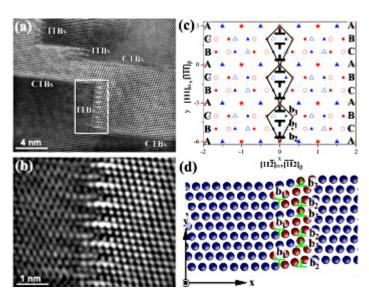


Figure 1 (a): HRTEM micrograph of grain boundaries. (b) Magnified HRTEM micrograph showing narrow and straight $\Sigma 3\{112\}$ ITBs. (c) Dichromatic pattern of a [110] $\Sigma 3\{112\}$ \|\{112\} twin boundary showing the atomic structure of the boundary consisting of a unit of three {111} planes and the corresponding Shockley partial dislocations. (d) The relaxed atomic structure by using atomistic simulation.

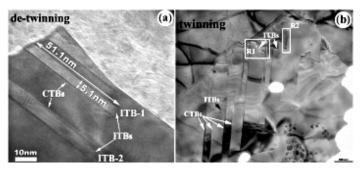


Figure 2 (a): In situ HRTEM observation of detwinning in Cu via the collective glide of the ITBs. (b) The HRTEM observation of twinning in Ag through the collective glide of the ITBs.

processes transform the interface plane from {111} to {100}, in agreement with experimental observation [*Int. J. Plasticity* **27** 121 (2011), *Scripta Mater* **64** 1083 (2011)]. Interface-driven twinning as revealed by this study suggests the exciting possibility of altering the roles of dislocation slip and twinning through the design of hetero-phase interface structure and properties.

This work was supported as part of the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number 2008LANL1026.

Technical contacts: Jian Wang, Amit Misra and Irene J Beyerlein

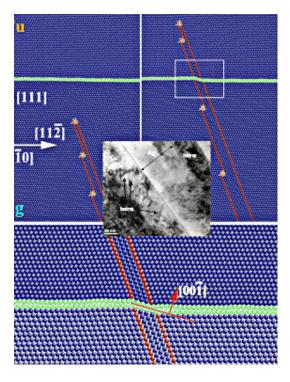


Figure 3: Interface-facilitated twinning in Cu through the twin transmission across the Cu-Ag interface. Atomistic simulations show the initial, final, and the magnification of the twin transmission region. TEM image shows the fine twins in Cu.

Using advanced characterization techniques to probe damage evolution

Developing the relationship between damage evolution and microstructure is critical to the formulation and validation of improved predictive models of the damage and failure process in polycrystalline materials.

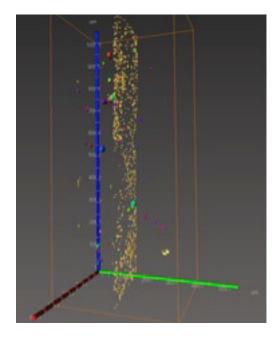
In a recent study Los Alamos researchers applied several characterization techniques to measure local strain fields with respect to microstructural features in a coarse-grained aluminum sample.

The primary goal is to quantify the effect of the spatial location of damage sites, with respect to local microstructure, on the incipient stages of damage localization. A secondary objective is to correlate surface and internal strain measurements via the digital image correlation (DIC) technique.

Initial results from this investigation are provided by an aluminum tensile sample that incorporates a pre-existing porosity damage field. This sample is fabricated via diffusion bonding with an internal surface accessible to DIC strain measurements.

Applied characterization techniques include electron backscatter diffraction (EBSD), DIC, and x-ray computed microtomography (XCMT). Following EBSD orientation mapping of the initial state, the external surface strain field is measured by DIC in situ during interrupted uniaxial tensile testing, while the internal void structure and internal surface displacements are determined ex situ by XCMT following each strain increment.

This novel technique allows for the non-destructive tracking of localized internal strains while also imaging the evolving internal damage state. Preliminary results are shown in the accompanying



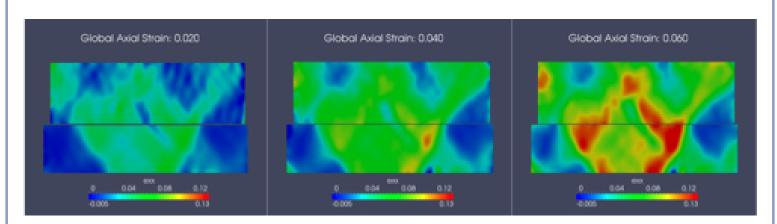
False-color XCMT image from a diffusion bonded aluminum tensile sample. Multi-colored globular shapes represent internal porosity inherited from the casting process, while gold particles are the tungsten tracers along the diffusion-bonded interface.

figures of the initial void field and distribution of tracer particles, along with local strain maps as a function of global strain. Local strains range from 2% to 15% at 6% total strain, providing correlation between the initiation and development of strain gradients with microstructural features.

Researchers include Matthew Tucker (MST-8/Gas Transfer Systems, W-7), John Bingert and Cheng Liu (MST-8), Brian Patterson, (Polymers and Coatings, MST-7), and Manny Lovato (MST-8).

This effort is supported by Science Campaign 2 and the DoD/DOE Joint Munitions Program.

Technical contacts: Matt Tucker and John Bingert.



Maps of localized strains parallel to axial loading from DIC measurements on two external surfaces, as a function of global strain.

Condensed matter physics conference features plenary talk by Gray

Rusty Gray (MST-8) recently presented the plenary talk at the 2011 American Physical Society Topical Conference on the Shock Compression of Condensed Matter in Chicago.



In his talk, Gray discussed the steps required to attaining a predictive capability that enables accurate simulations of

dynamic impact, shock, and high-rate loading phenomena applications. In particular, he called for a linked experimental, modeling, and validation research program, stressing that only by close collaboration between experimentalists and modelers can the derivation of physically based materials models be achieved.

A fellow of the American Physical Society and past president of The Minerals, Metals & Materials Society, Gray received his doctorate from Carnegie Mellon University. He joined the Laboratory in 1985. The Topical Group on Shock Compression and Condensed Matter promotes the development and exchange of information on the dynamic high-pressure properties of materials. The conference attracts 500 attendees from a variety of countries, institutions, and industries.

Technical contact: Rusty Gray

Celebrating service

Congratulations to the following MST employee celebrating a service anniversary this month:

Joseph Baiardo, MST-16

25 years



Published monthly by the Experimental Physical Sciences Directorate. To submit news items or for more information, contact Karen Kippen, EPS Communications, at 606-1822, or kkippen@lanl.gov.

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HeadsUP!

Safety reminder: School starts this month

Practice safety in school zones

This month, many students are returning to classrooms throughout Northern New Mexico. Employees and the public are reminded to practice safety in and around school zones and neighborhoods. Here are some tips:

When driving:

- Slow down and be especially alert in the residential neighborhoods and school zones
- Take extra time to look for children at intersections, on medians and on curbs
- · Enter and exit driveways and alleys slowly and carefully
- Watch for children on and near the road in the morning and after school hours
- Reduce distractions inside your car and concentrate on the road and your surroundings
- · Don't talk on cell phones or text while driving.
- Use turn signals to announce your intent when pulling into the school parking lot or to the side of the road.

Remind student pedestrians to....

- Cross the street at corners, using traffic signals and crosswalks
- Never run out into the streets or cross in between parked cars
- Make sure to always walk in front of the bus where the driver can see you.

New tool for emergency notifications

If a situation exists at the Lab requiring emergency notification, employees soon will be contacted through the Lab's new Mass Notification System. The Mass Notification System is web-based and able to send out emergency life-saving instructions. Beginning the week of August 22, select populations and locations will receive test messages.

The system's contact information is populated from the Oracle database and is dependent on the accuracy of Oracle information. If you have not updated your information in Oracle, please do so now. See Oracle Applications under "Top Tools" on the LANL homepage (int.lanl.gov).